ADMET Group Leaderboard

References

Submission Instructions

BenchmarkGroup Class Documentation

Leaderboard Guidelines

`TDC.Caco2_Wang` Leaderboard

Dataset Summary

Dataset	Unit	Size	Task	Metric	Dataset Split
TDC.Caco2_Wang	cm/s	906	Regression	MAE	Scaffold

Leaderboard

Rank	Model	Contact	Link	#Params	MAE ⬇
1	MapLight	Jim Notwell	GitHub, Paper	N/A	0.276 ± 0.005
2	BaseBoosting	Andrew Li	GitHub, Paper	365,713	0.285 ± 0.005
3	MapLight + GNN	Jim Notwell	GitHub, Paper	N/A	0.287 ± 0.005
4	MolMapNet-D	Shen Wan Xiang	GitHub, Paper	407,617	0.287 ± 0.005
5	XGBoost	Andrew Li	GitHub, Paper	12	0.289 ± 0.011
6	Basic ML	Nilavo Boral	GitHub, Paper	N/A	0.321 ± 0.005
7	Chemprop-RDKit	Kyle Swanson	GitHub, Paper	N/A	0.330 ± 0.024
8	CFA	Nan Jiang	GitHub, Paper	N/A	0.335 ± 0.033
9	Euclia ML model	Euclia	GitHub, Paper	50	0.341 ± 0.004
10	Chemprop	Kyle Swanson	GitHub, Paper	N/A	0.344 ± 0.015
11	RDKit2D + MLP (DeepPurpose)	Kexin Huang	GitHub, Paper	633,409	0.393 ± 0.024
12	AttentiveFP	Kexin Huang	GitHub, Paper	300,806	0.401 ± 0.032
13	CNN (DeepPurpose)	Kexin Huang	GitHub, Paper	226,625	0.446 ± 0.036
14	ContextPred	Kexin Huang	GitHub, Paper	2,067,053	0.502 ± 0.036
15	NeuralFP	Kexin Huang	GitHub, Paper	480,193	0.530 ± 0.102
16	AttrMasking	Kexin Huang	GitHub, Paper	2,067,053	0.546 ± 0.052
17	GCN	Kexin Huang	GitHub, Paper	191,810	0.599 ± 0.104
18	Morgan + MLP (DeepPurpose)	Kexin Huang	GitHub, Paper	1,477,185	0.908 ± 0.060

⬇: The lower the better.